Computational Chemistry for Better Batteries

***Objective*: Predict & optimize the structure of fluid-solid electrolyte interfaces that are important in future energy technologies**

***Implications*: Lithium-ion batteries are an example; finding the right electrolyte for them could revolutionize transportation.**

***Accomplishments:* Used molecular dynamics simulation to determine, for the first time, accurate solvation models, diffusion coefficients, and solvation energies for lithium ion in two contrasting electrolytes.**

- **Another key example of simulation/ experiment interplay; helps explain neutron, X-ray, NMR, and optical data.**
- **Simulations are more accurate than "classsical" simulations and agree well with experiments.**

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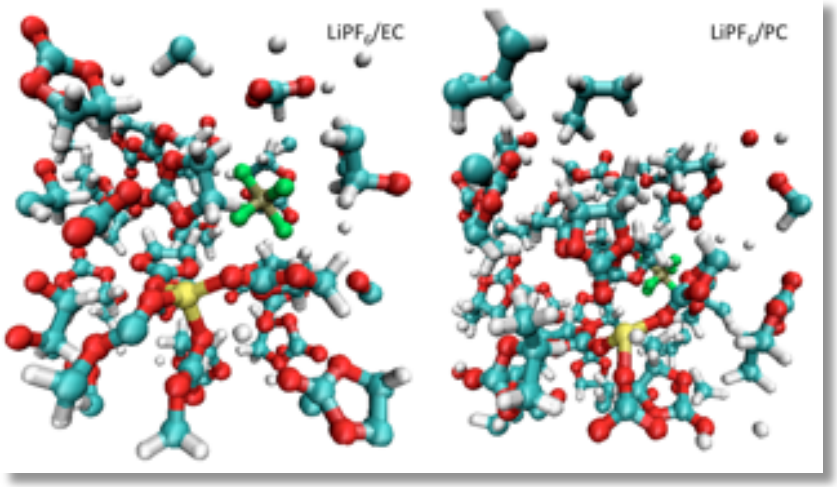

Simulation results for lithium ion in two solvents, ethylene-carbonate (left) and propylene-carbonate (right).

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